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An Improved Hybrid Monte Carlo Method

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Abstract

The hybrid Monte Carlo algorithm does not completely remove problems with ergodicity in the molecular dynamics trajectories unless the length of each trajectory, τ_0, is kept shorter than the period of the fastest mode of the system, $2\pi/\omega_{max}$. The correlations which remain when larger values of τ_0 are used may be eliminated by randomizing not only the molecular dynamics velocities but also the length of the trajectory, τ_0, at the beginning of each new trajectory. This allows τ_0 to be increased to the time scale of the slowest modes in the system, $1/\omega_{min}$, and reduces the correlation time (and therefore the computer time used) by a factor of around $\omega_{max}/2\omega_{min}$.

The most efficient existing algorithm for solving Quantum Chromodynamics (QCD) numerically on a discrete lattice is the hybrid Monte Carlo[1] algorithm. Monte Carlo simulation algorithms such as this one are designed to produce a sequence of configurations of the fields ϕ with a probability distribution which approaches $\exp(-S(\phi))$, where $S(\phi)$ is the action of the theory. This particular algorithm evolves the fields on each sweep by an amount proportional to a small step size, dt, unlike the metropolis and heat bath algorithms which update the fields one lattice site at a time by as large a step size as possible. It introduces a new fictitious time coordinate and fictitious velocities π conjugate to the field variables which are evolved by Hamilton's equations using the Hamiltonian $H = S(\phi)+\Sigma\pi^2/2$. After some fixed length of molecular dynamics time τ_0, the velocities are randomized using the probability distribution $\exp(-\Sigma\pi^2/2)$ to ensure the correct probability distribution for the ϕ fields, and to try to ensure ergodicity. For QCD calculations including the effects of the sea quarks, small step size algorithms are preferred to the large step size algorithms because they require the time consuming calculation

of a quark propagator once per sweep of the entire lattice rather than once for every update of a single site.

An empirical rule of thumb is sometimes given that the hybrid Monte Carlo algorithm appears to have roughly the same decorrelation time in molecular dynamics time units as the Metropolis algorithm has in sweeps.[2] This is disappointing and puzzling. In free field theory, the action is diagonal in the Fourier transformed lattice fields: $S = \Sigma_p(\Sigma_\mu \sin^2(p_\mu/2) + m^2)\phi_{-p_\mu}\phi_{p_\mu} \equiv \Sigma_{p,\mu}\, \omega^2_{p_\mu}\phi_{-p_\mu}\phi_{p_\mu}$. The low momentum modes undergo larger fluctuations than the high momentum modes. The step size of the Metropolis algorithm is limited by the requirement that the steps, which affect all modes equally, not drive the high momentum modes out of equilibrium. They therefore produce only small changes in the low momentum modes, which require many sweeps (of order $(\omega_{max}/\omega_{min})^2$) to random walk to a new value.

Hybrid algorithms by contrast evolve the fields during a trajectory in a more direct path, rather than by a random walk. It might therefore have been hoped that by choosing the trajectory length τ_0 to approach the time scale of the slowest modes of the system, all of the modes could be randomized after a single trajectory, which would lead to a correlation time in sweeps of order $1/(\omega_{min}dt)$. In practice, it has usually been found that the algorithms perform better with τ_0 around 1 or 2 times $1/\omega_{max}$. This randomizes the fast modes after a single trajectory, but requires $(\omega_{max}/\omega_{min})^2$ trajectories to randomize the slow modes, leading to correlation times in sweeps of order $(\omega_{max}/\omega_{min})^2/(\omega_{max}dt)$.

The problem is illustrated in Figure 1. It shows the evolution of the action of a free scalar field with the hybrid Monte Carlo algorithm on an 8^4 lattice. The parameters used were m=0.2 and dt=0.1. τ_0 was taken to be $1/\omega_{min} = 1/m = 5.0$. This is a seemingly reasonable value from the standpoint of optimizing the relaxation over the slowest mode, but it turns out to be a spectacular failure in this case. The correct equilibrium value for the action in this system is $S = 2048$. The simulation was started far from equilibrium to make the effect stand out. The peaks in the figure every 50 sweeps occur at the refreshes of the momenta. The figure shows that after the first molecular dynamics trajectory, at the beginning of each trajectory the system relaxes closer to its equilibrium value, and then just as the velocities are about to be refreshed, jumps back to close to its starting value. It can be seen that there are correlations which last far longer than τ_0. The action does not reach its equilibrium value after even hundreds of trajectories (tens of thousands of sweeps).

Setting τ_0 to a different value or adding an interaction term to the action do not qualitatively change the effect until τ_0 approaches $1/\omega_{max}$. This is not simply a pathology of the free field theory. In the simulation shown in Figure 2, a $\lambda\phi^4$ interaction with $\lambda = 0.1$ has been added to the action. All the other parameters of the run were left unchanged, including the random number

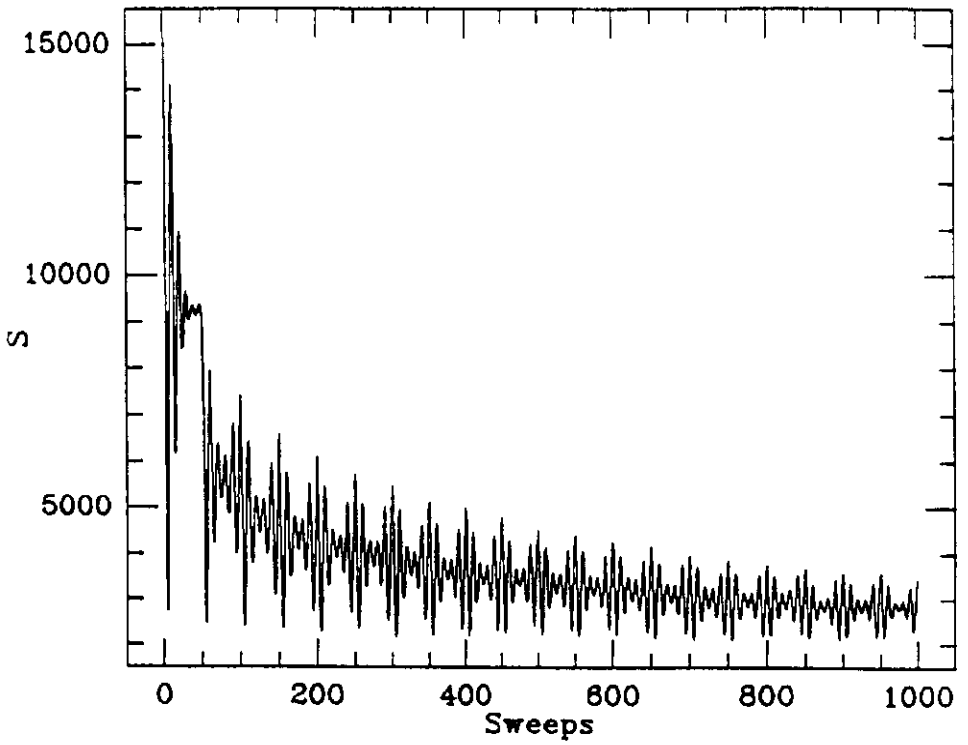

Figure 1: The evolution of the action of a free scalar field on an 8^4 lattice using the hybrid Monte Carlo algorithm. The velocities are refreshed every 50 sweeps. When the simulation is started far from the equilibrium action of $S = 2048$, it can be clearly seen that during each trajectory, the action approaches closer to its equilibrium value, but then jumps back almost to its starting value just as the velocities are about to be refreshed. This effect is not sensitive to small changes to the trajectory length or to the addition of small interaction terms.

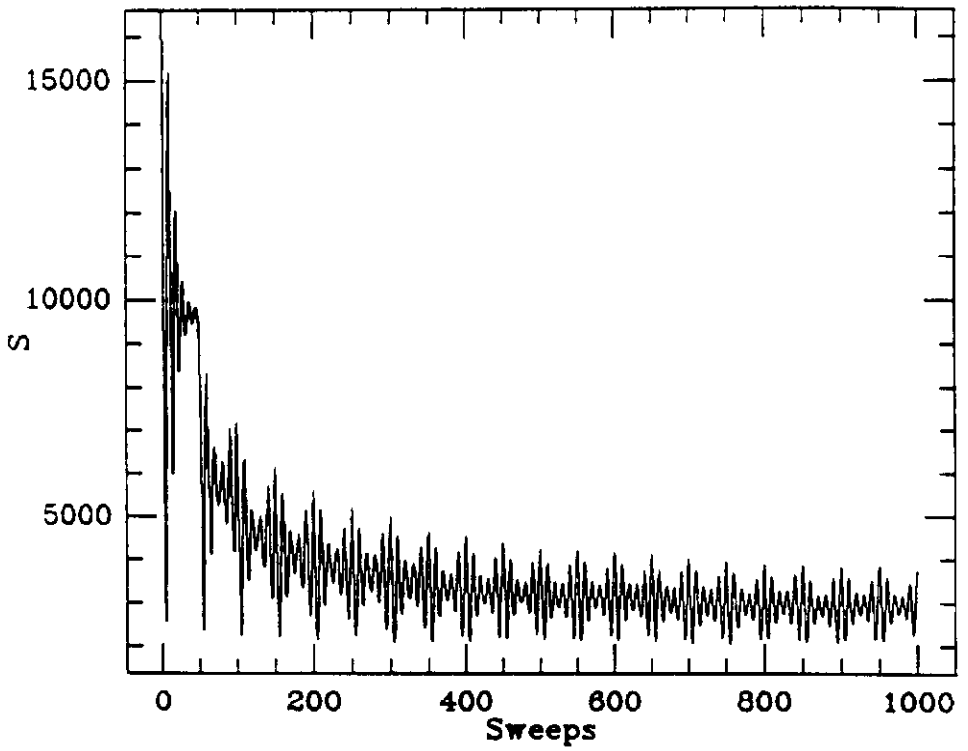

Figure 2: The same as Figure 1, except that a $\lambda\phi^4$ interaction with $\lambda = 0.1$ has been added to the action. The effect seen in Figure 1 is qualitatively unchanged.

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The effect can be understood by looking at Figure 3. The top graph shows the distribution of periods for the microcanonical evolution of the normal modes of a free scalar field on an 8^4 lattice with $m = .2$. The bottom graph shows all integer multiples of the periods less than or equal to T_{max}. It can be seen that for any value of τ_0 larger than $T_{min} = 2\pi/\omega_{max}$, there are likely to be some modes satisfying $|n(2\pi/\omega) - \tau_0| < \epsilon$ which evolve by an amount $\epsilon\omega$ under the microcanonical trajectory. (ϵ in this case is roughly .05.) These modes will take of order $(\epsilon\omega)^{-2}$ trajectories to random walk one radian away from their starting points. This in not simply a matter of hitting a resonance by bad luck; the modes are quite dense. Since the density of frequencies increases as the volume of the lattice, these correlation times tend to grow as the lattice volume squared.

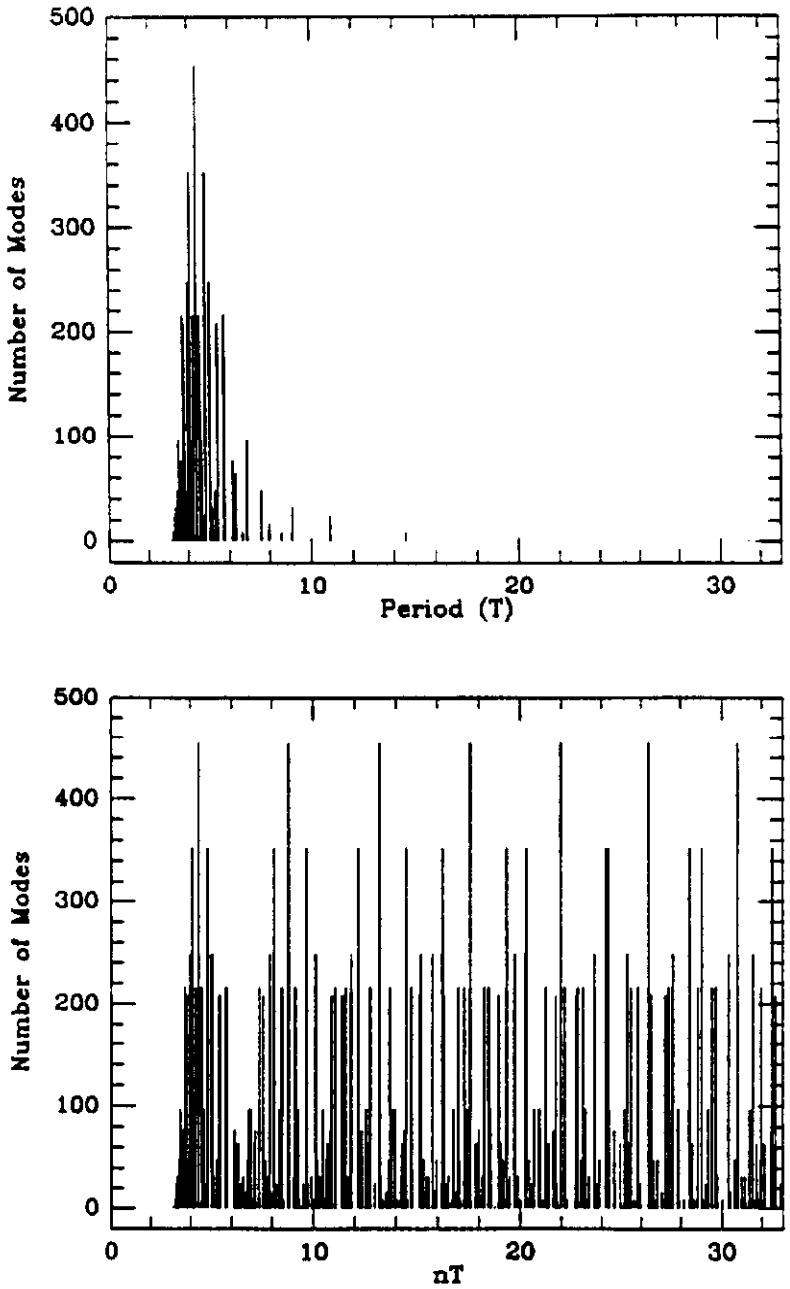

Figure 3: The top figure shows the distribution of periods of the modes of a free scalar field with $m = 0.2$ on an 8^4 lattice. The bottom figure shows the distribution of integer multiples of these periods with $nT < T_{max}$. For any τ_0 larger than T_{min}, there will be some modes with nT very close to τ_0. These modes will change very little under a molecular dynamics trajectory of length τ_0.

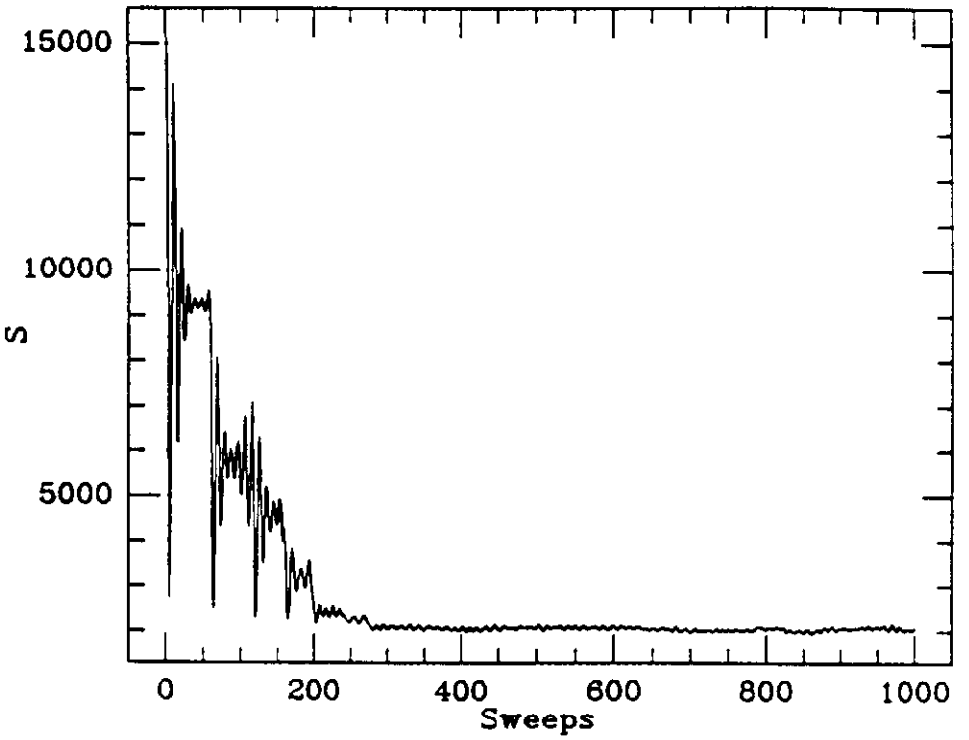

Figure 4: The same as Figure 1, except that the length of each trajectory is varied randomly between 35 and 65 sweeps. In this case, the action approaches its equilibrium value after only a few trajectories. Different modes satisfy $nT \approx \tau_0$ on different trajectories.

To remove these remaining correlations, it is necessary to vary τ_0 at each new microcanonical trajectory. In this way, a different set of modes will be left unrandomized by each new trajectory. This may be done by varying dt, the number of steps, or both. Figure 4 is the same as Figure 1 except that τ_0 is varied randomly from $.7/\omega_{min}$ to $1.3/\omega_{min}$ by varying the number of steps. In this case, the action reaches its equilibrium value after only a few trajectories. Requiring further investigation are the question of the optimal range of variation of τ_0 and the question of whether it is better to vary the number of steps, the step size, or both.

The effect discussed here does not occur in the original hybrid algorithm of Duane and Kogut[3], which had a varying trajectory length built into it. Interactions help the ordinary hybrid Monte Carlo method perform a bit better for large trajectory length, but the algorithm still performs best when $\tau_0 < 2\pi/\omega_{max}; \tau_0 \approx 2/\omega_{max}$ is often near the optimum value. This leads to an expected improvement using the algorithm of this paper of around $\omega_{max}/(2\omega_{min})$, which may amount to a factor of 3-5 for QCD simulations near the continuum limit.

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References

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